

2021 DOE Vehicle Technologies Office  
Annual Merit Review

## Fuel Effects on Multimode Engine Operation

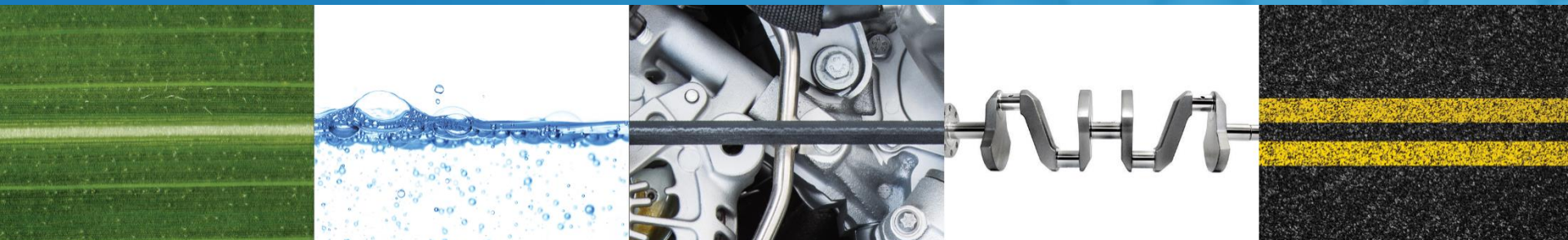
Magnus Sjöberg  
Sandia National Laboratories  
Project ID # FT092

June 24 - 2021

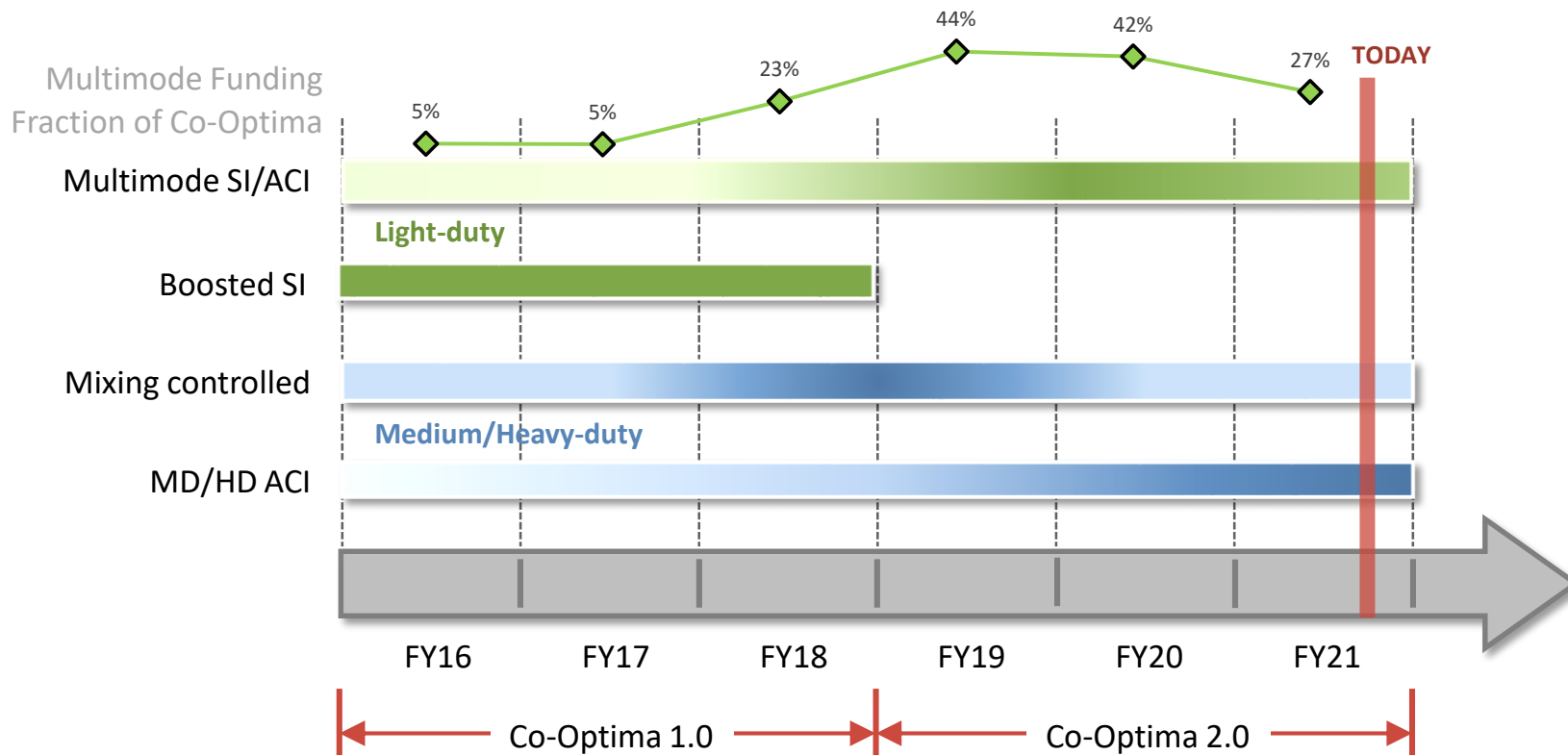


CO-OPTIMIZATION OF  
**FUELS & ENGINES**

better fuels | better vehicles | sooner



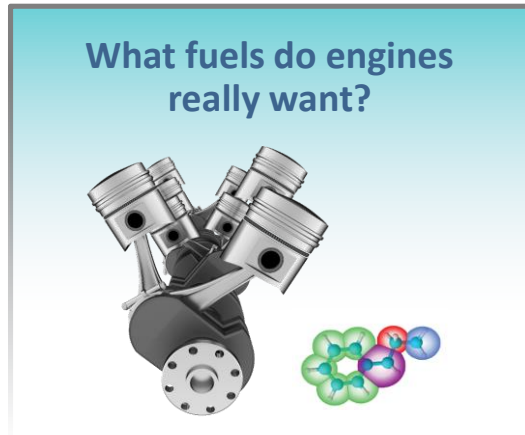
# Overview | Timeline



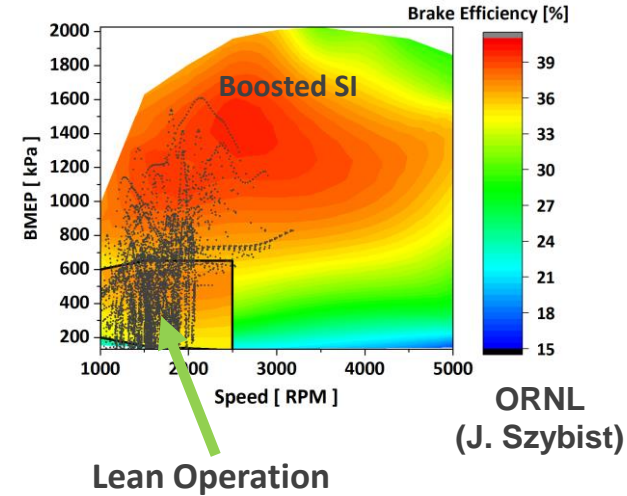
# Introduction



- Focus is on Light-duty Multimode (MM) engine operation.
- MM uses advanced combustion at lower loads in combination with boosted SI at high loads.
- Here, sampling from Co-Optima efforts on MM.
  - Highlight the role of important fuel properties.



- MM fuels need to enable Boosted SI.



- Provide quantitative example of how MM can provide fuel-economy benefits.

# Contributions from Across Co-Optima Teams



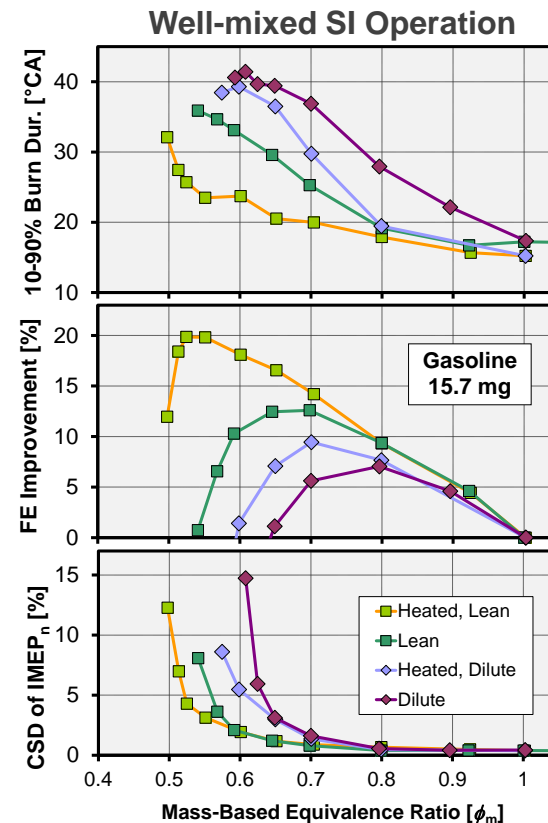
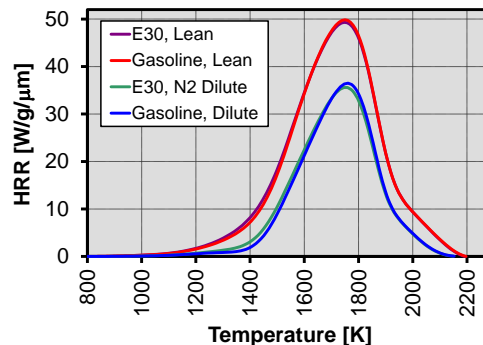
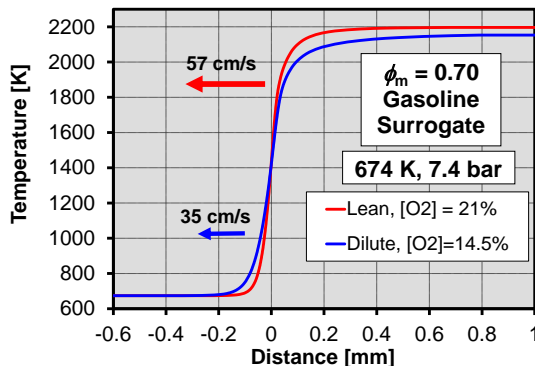
Only a small fraction of all Multimode work is featured in this presentation.

This research was sponsored by the U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE), Bioenergy Technologies and Vehicle Technologies Offices.

# Benefits and Challenges with Lean Operation



- Increased thermal efficiency.
  - Increased  $\gamma$ , reduced pumping losses and heat transfer.
- Combustion instability.
- Excessive burn duration.
- Lean  $\text{NO}_x$  aftertreatment.
- Dilute well-mixed SI:
  - 3-way catalyst can be used.
  - Slow combustion and limited FE gain.



SNL (M. Sjöberg) – [1]

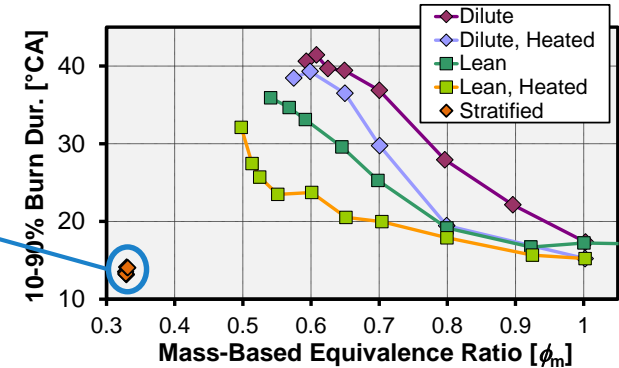
LLNL (W. Pitz and M. Mehl)

# Benefits and Challenges with Lean Operation (2)

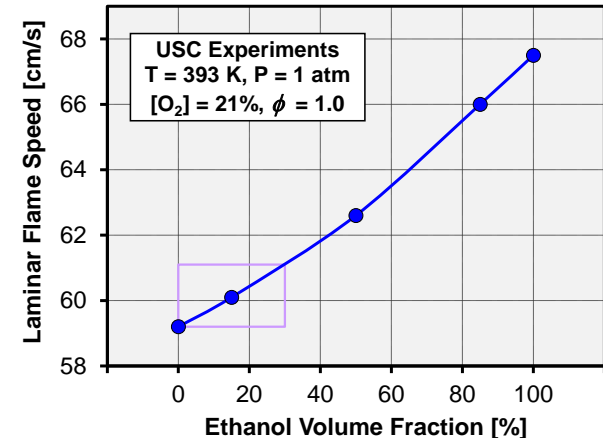


- Increased thermal efficiency.
  - Increased  $\gamma$ , reduced pumping losses and heat transfer.
- Combustion instability.
- Excessive burn duration.
- Lean  $\text{NO}_x$  aftertreatment.
- Dilute well-mixed SI:
  - 3-way catalyst can be used.
  - Slow combustion and limited FE gain.
  - Fuels with inherent high flame speed are beneficial, but limited opportunities with the maximum 30% blend level of Co-Optima.
- ACI (advanced compression ignition) techniques can enable fast burn even for very lean conditions.
- Also fully stratified-charge (SC) SI enables lean burn.
  - Multiple bioblendstocks provide fast combustion.

Regular Gasoline - RD5-87  
Ethanol - E30  
Di-isobutylene  
Iso-Butanol  
2-butanol



SNL (M. Sjöberg)

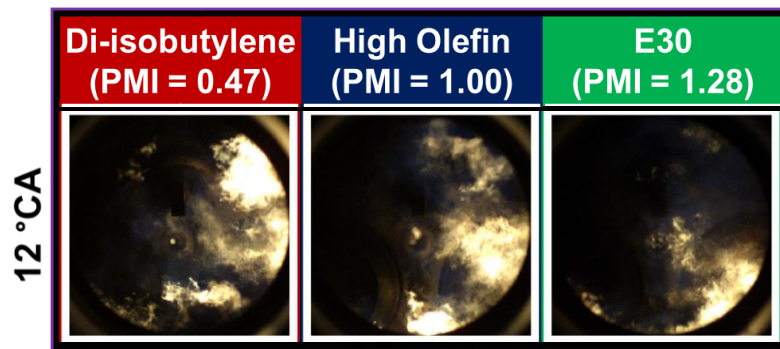
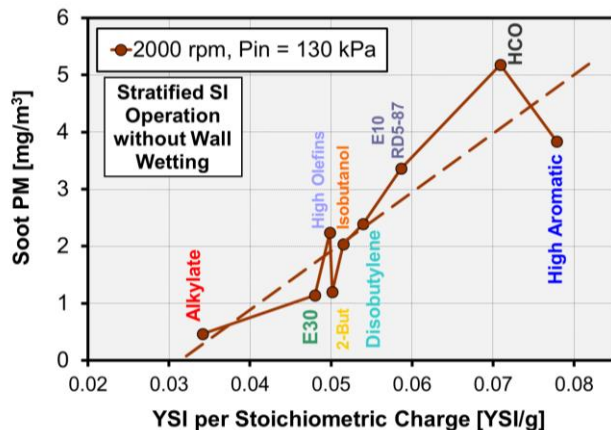
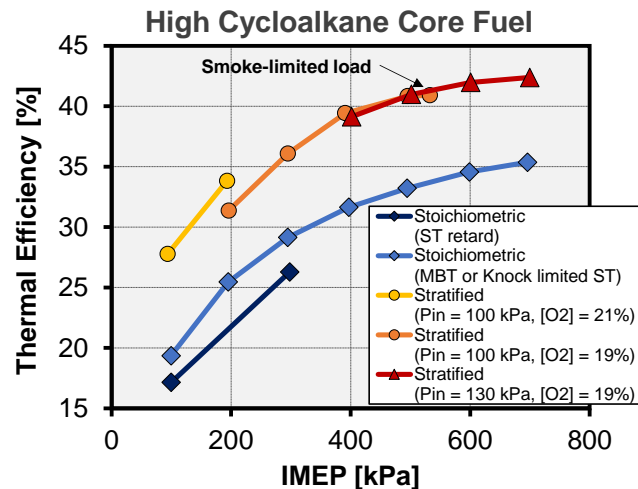


USC (R. Zhao & F. Egolopoulos)

# Overcoming Challenges with Lean Operation; Role of Fuel Properties for Stratified-charge (SC) SI



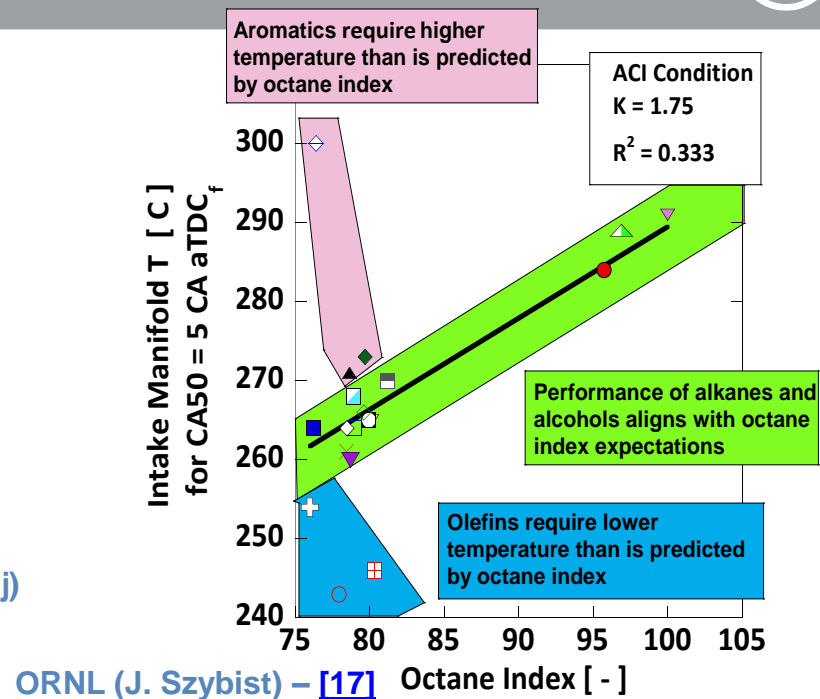
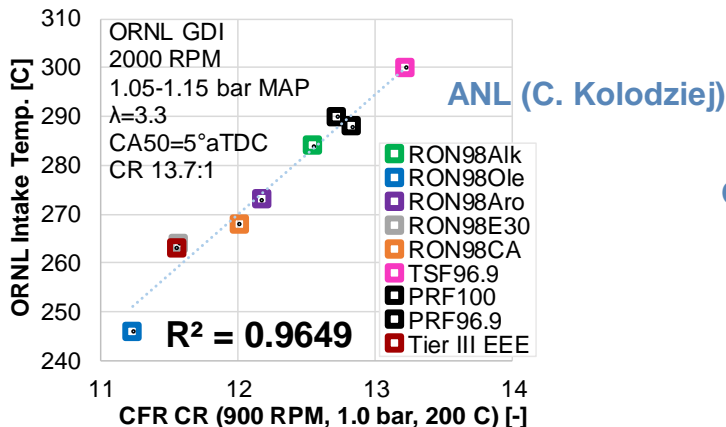
- **Superior thermal efficiency.**
- **Load can be smoke limited**, especially when EGR is used to suppress  $\text{NO}_x$ .
- Fuels with low sooting propensity are desirable.
- But common sooting metrics not always applicable.
- New sooting metrics are being considered.
  - Collaboration with Yale (C. McEnally) and LLNL (S. Lapointe [\[23\]](#)).



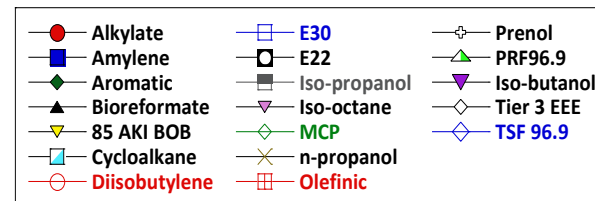
# Overcoming Challenges with Lean Operation; Role of Fuel Properties for HCCI



- **Low  $\text{NO}_x$ .**
- **Requires high reactant temperatures**, which decreases  $\gamma$  & increases heat transfer.
- **Combustion-phasing control challenge.**
- RON & MON often inadequate for  $K > 1 \Rightarrow$  use compositional constraints or newly developed CFR HCCI rating.



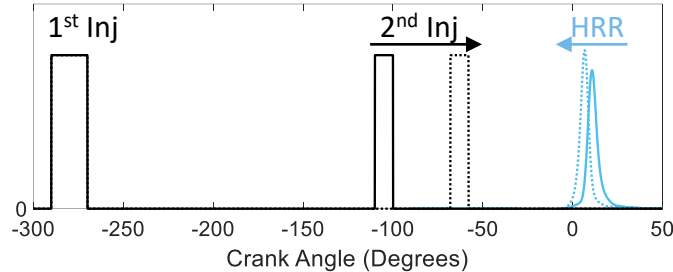
ORNL (J. Szybist) – [17]



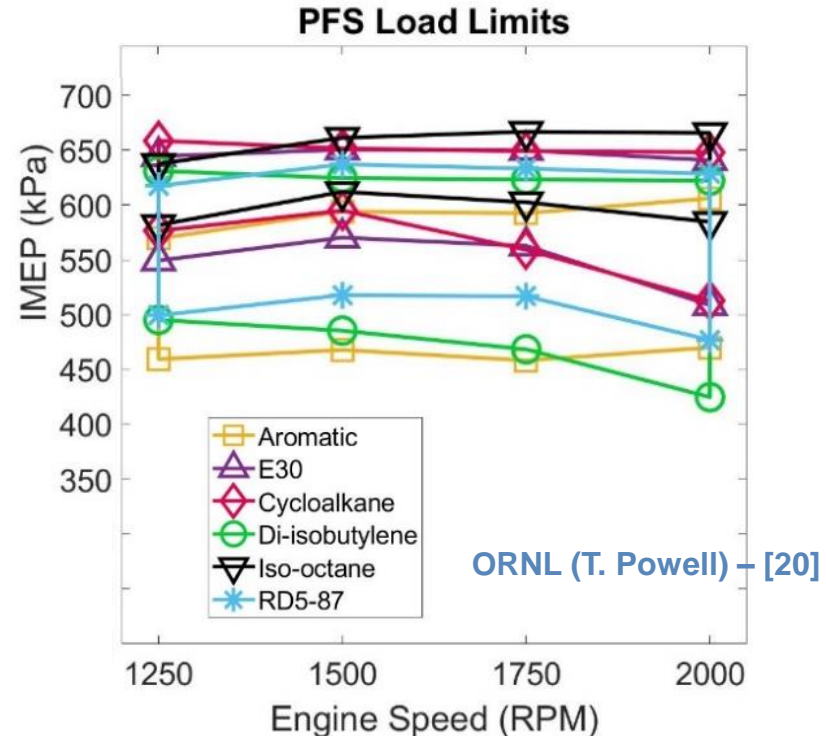
# Overcoming Challenges with Lean Operation; Role of Fuel Properties for PFS-ACI



- Uses stratification to aid combustion control.



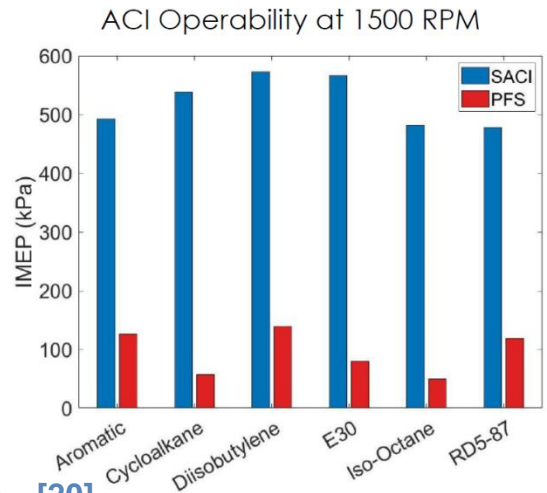
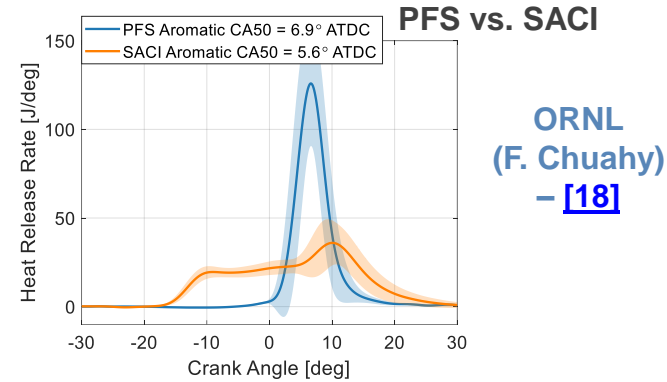
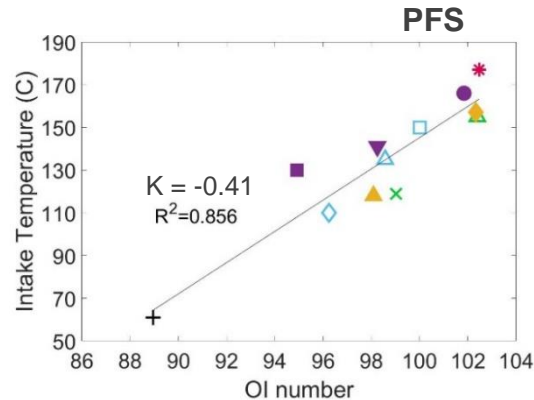
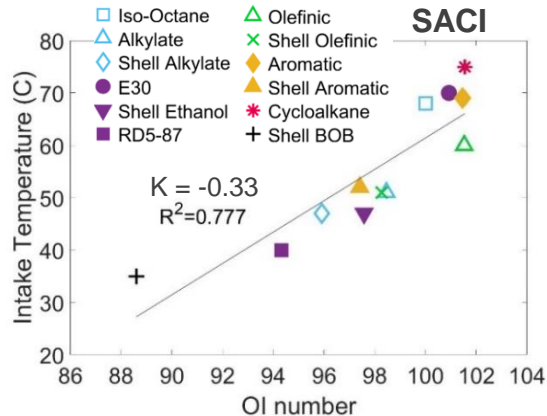
- Requires high boost pressure for CRs suitable also for boosted SI.
- Limited load range.
- Lower load limits (defined by  $CE > 92.5\%$ ) varies with fuel.
  - Di-isobutylene and Aromatic fuels best at maintaining high combustion efficiency (CE).
  - Fuel properties do not explain these differences.
- RON & MON generally applicable in terms of autoignition timing, see next slide.



# Overcoming Challenges with Lean Operation; Role of Fuel Properties for SACI



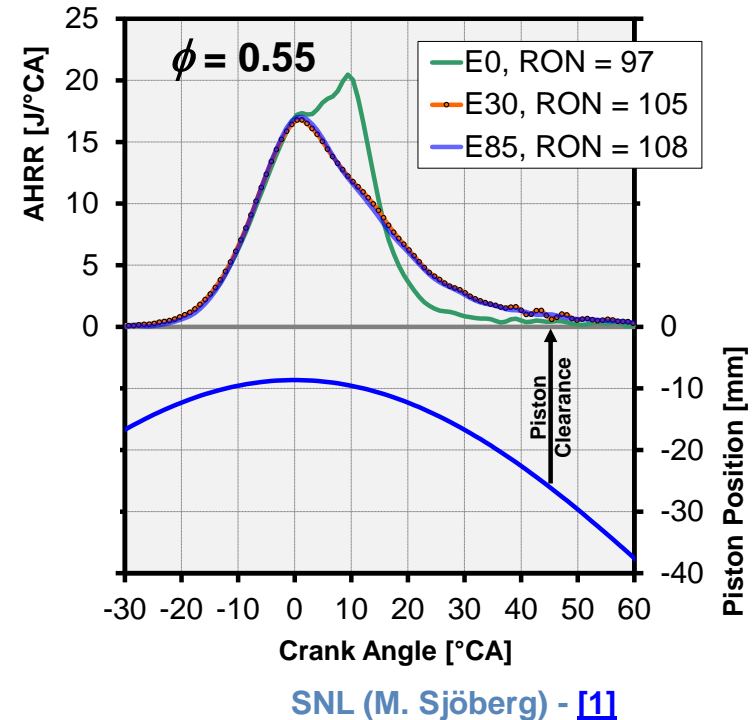
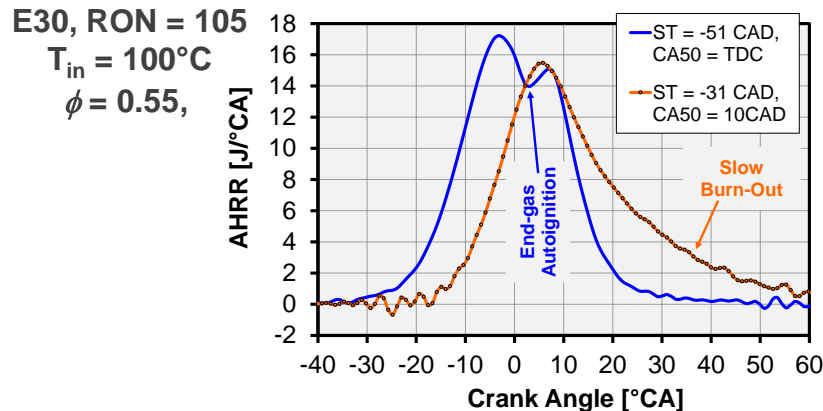
- Spark-timing controlled.
- Moderate reactant temperature requirement.
- Superior load range compared to PFS and HCCI.
- **Relatively high NO<sub>x</sub> levels** (but EGR helps).
- Mixed-mode combustion speeds up burn-out phase.
- RON and MON describe autoignition reactivity using Octane-Index (OI) framework for  $K < 1$



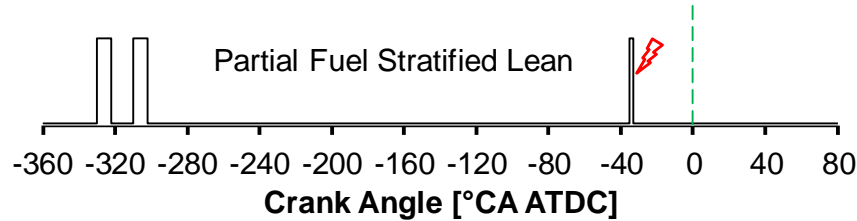
# An Examination of SACI; Well-Mixed SI Experiments



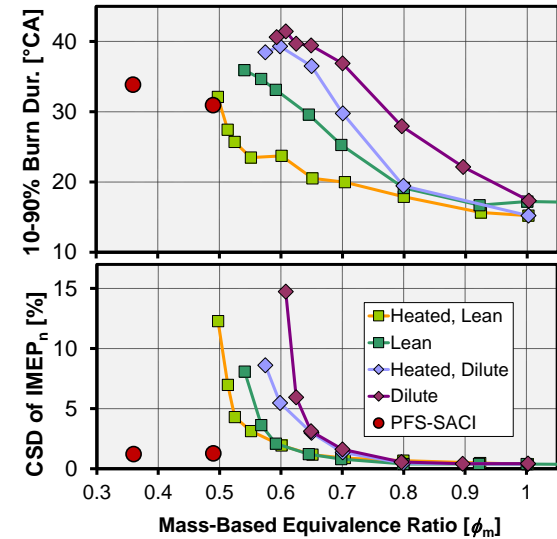
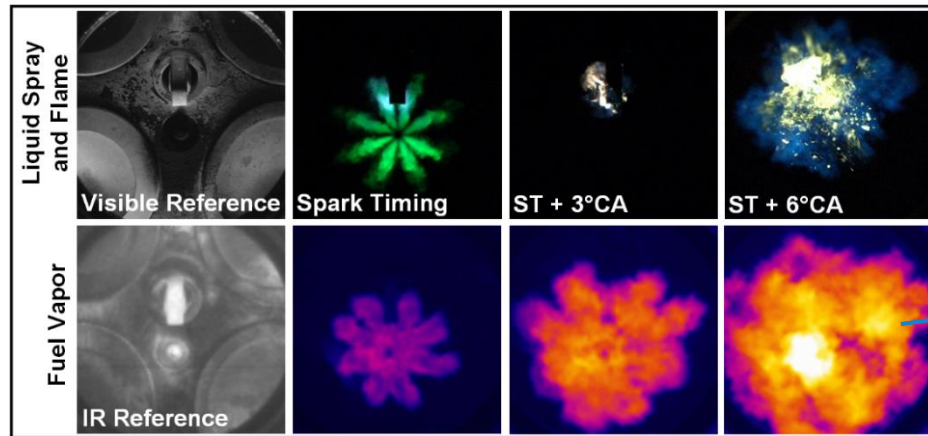
- Mixed-mode combustion speeds up burn-out.
- Deflagration  $\Rightarrow$  end-gas autoignition
- Ensures sufficiently short burn duration.
- For a given spark timing, induction of end-gas autoignition depends on the fuel.
- However, spark-timing adjustments can compensate for differences in fuel reactivity.



# An Examination of SACI; Partial Fuel Stratification (PFS) SI Experiments



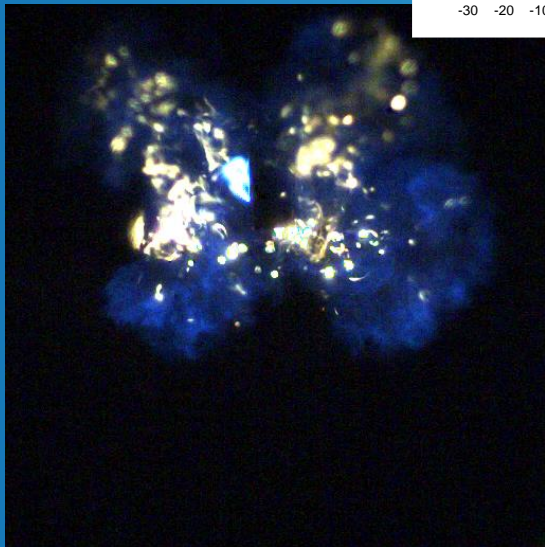
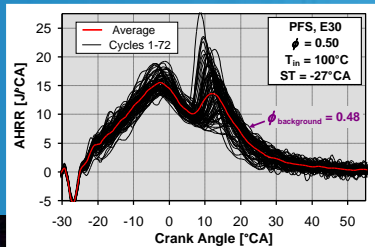
- To stabilize lean SACI operation, use pilot injection at the time of spark  $\Rightarrow$  PFS – SACI.



- Creates an enriched region near spark plug.
- Large 3.4 mg pilot in this example.

# PFS-SACI; Optical Imaging Experiments

- Smaller 0.7 mg pilot (210 $\mu$ s inj. dur.)
- Liquid fuel vaporizes quickly.



SNL (C. Tornatore) - [\[12\]](#)

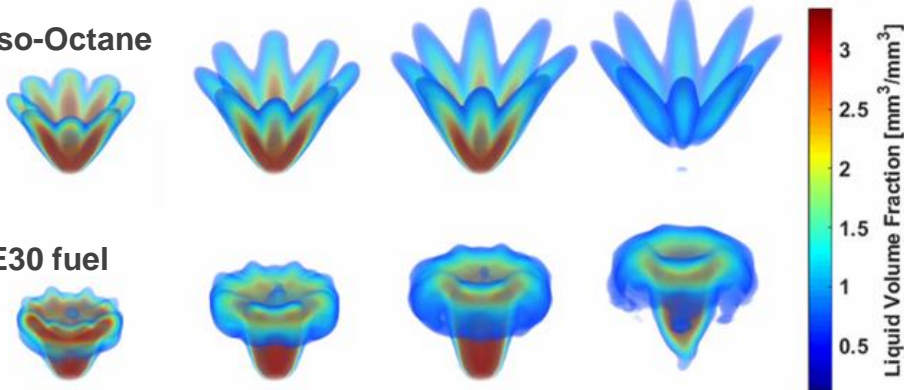
# Fundamental Spray Experiments



- PFS-SACI and PFS-ACI require good handle on fuel-air mixture formation.
- Spray-vessel experiments reveal strong influence of distillation curve on spray morphology at lower pressures.
  - Lower sensitivity for late injection.

## 3D Tomographic Images, P = 0.5 bar

iso-Octane



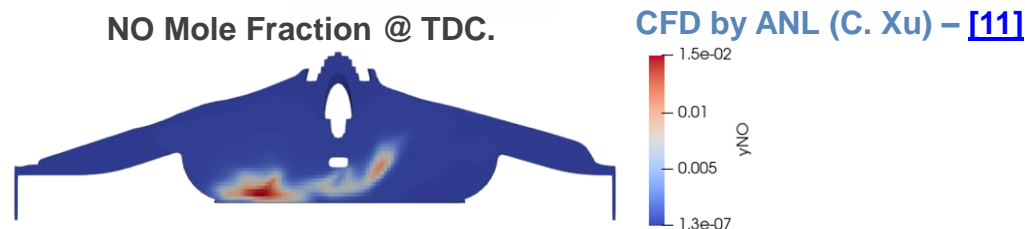
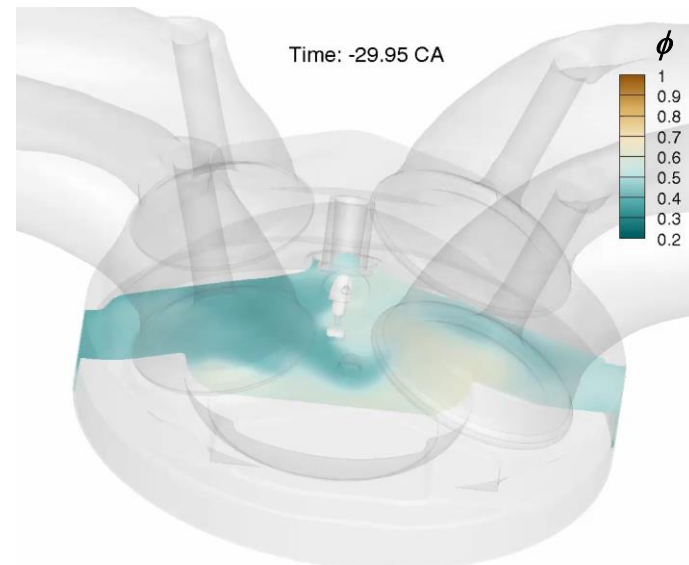
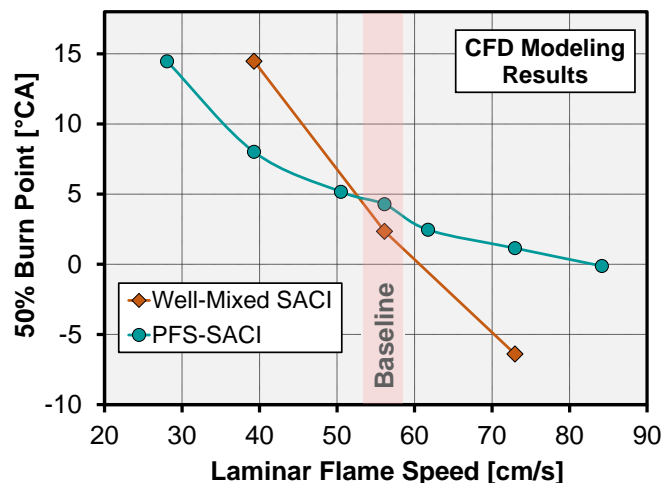
E30 fuel

SNL (J. Hwang) – [\[10\]](#)

# LES-CFD Reveals the Role of Flame Speed for SACI



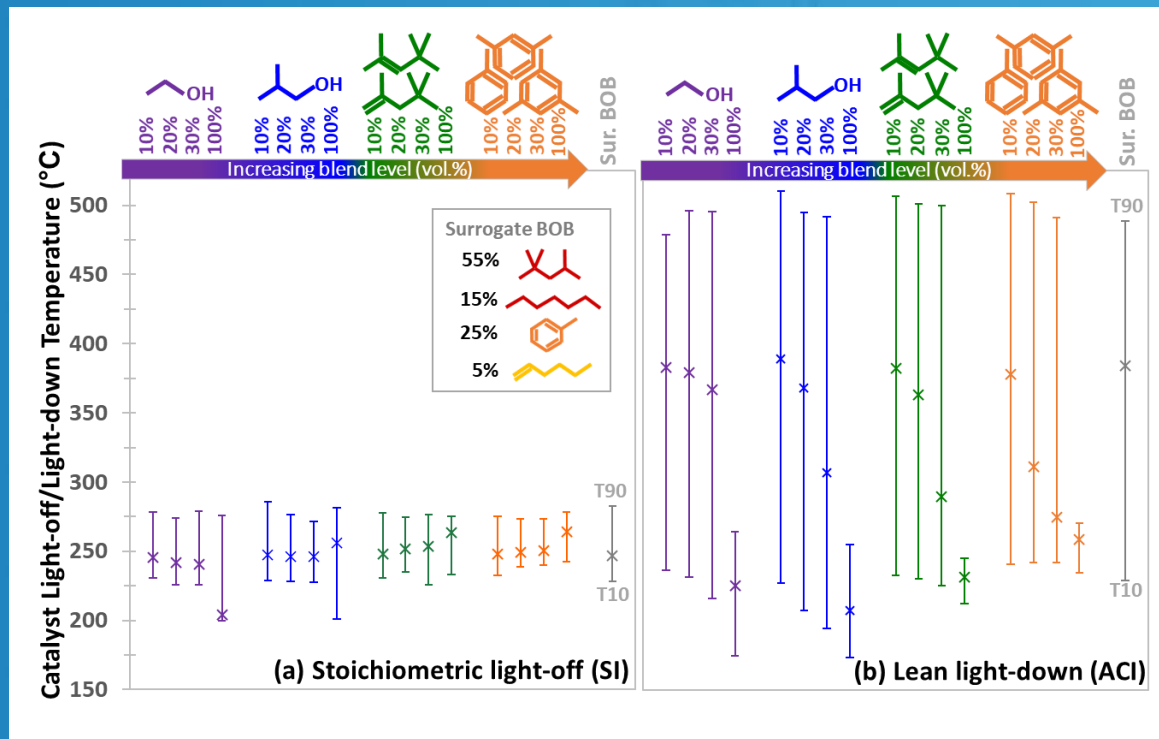
- Model predicts that PFS operation reduces sensitivity to variations of laminar flame speed.
- May enable PFS-SACI to provide stable operation with EGR to suppress  $\text{NO}_x$ .
- CFD reveals that  $\text{NO}_x$  formation is closely tied to mixture formation.



# Fuel Effects on Lean Exhaust Aftertreatment

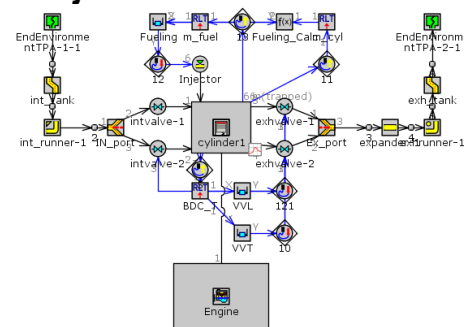
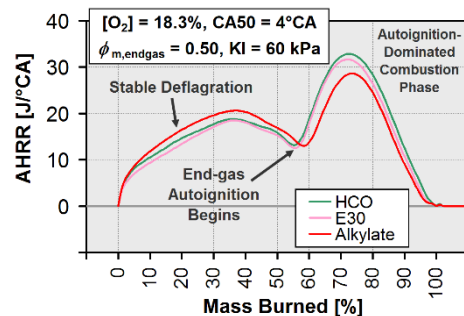
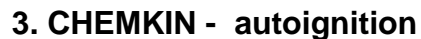


- Important to assess how bioblendstocks impact the performance of emissions control catalysts.
- Multimode engines must meet emissions regulations.
- Measured three-way catalyst (TWC) stoichiometric light-off and lean light-down temp.
- 10-30% blends of ethanol, isobutanol, di-isobutylene, and aromatics mixed into a surrogate BOB (+neat).
- Overall TWC reactivity is controlled primarily by the BOB components rather than the high performance blendstocks.





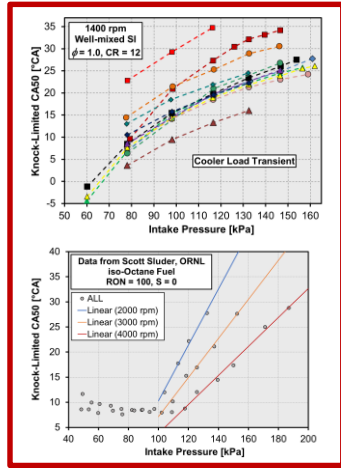
- ## 5. Quantify load ranges



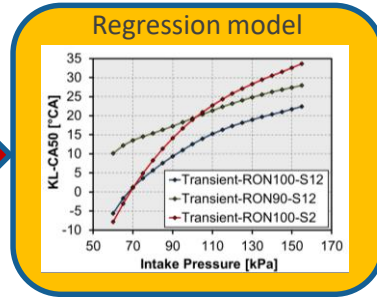
# Developed and Used Framework to Predict the Effect of Fuel Type on Fuel Economy; Stoichiometric and Multimode



Exp. Engine Data for many fuels, operating conditions & engine thermal states



Determine knock limits for hypothetical fuels



KL-CA50

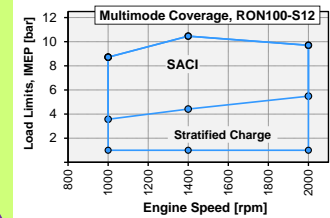
SNL (M. Sjöberg, N. Kim)  
LLNL (N. Killingsworth, M. McNenly)  
LBNL (J. Mueller)  
ANL (R. Vijayagopal)  
ORNL (S. Sluder)

Fuel Consumption Rate

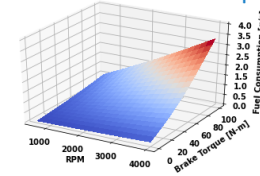
Gaussian Process Regression model

Torque, Fuel Flow

Multimode Coverage



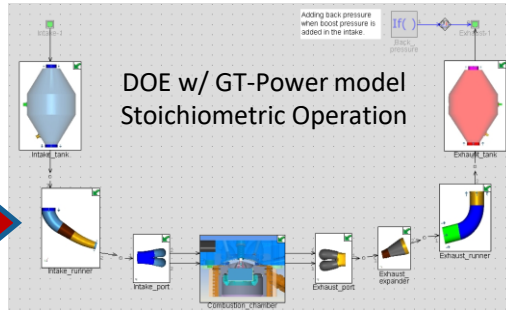
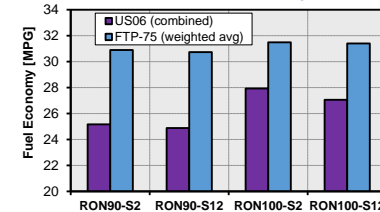
Fuel-Flow Rate Map



Drive Cycle Simulation

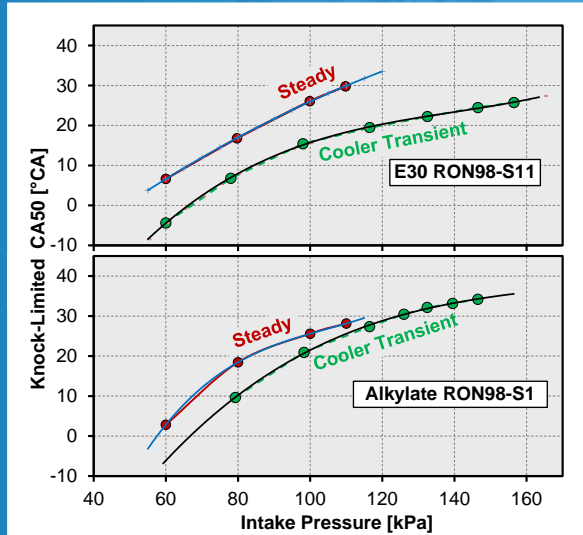


Fuel Economy



# Stoichiometric Knock Limits at Reduced Engine Thermal State

- High-power SI engine can benefit greatly from enhanced thermal management.
  - Suppression of engine knock. Especially important for downsized engines.
- Boosted knock limits of E30 are highly sensitive to the thermal state of the engine.
- Knock limits of Alkylate are much less sensitive.

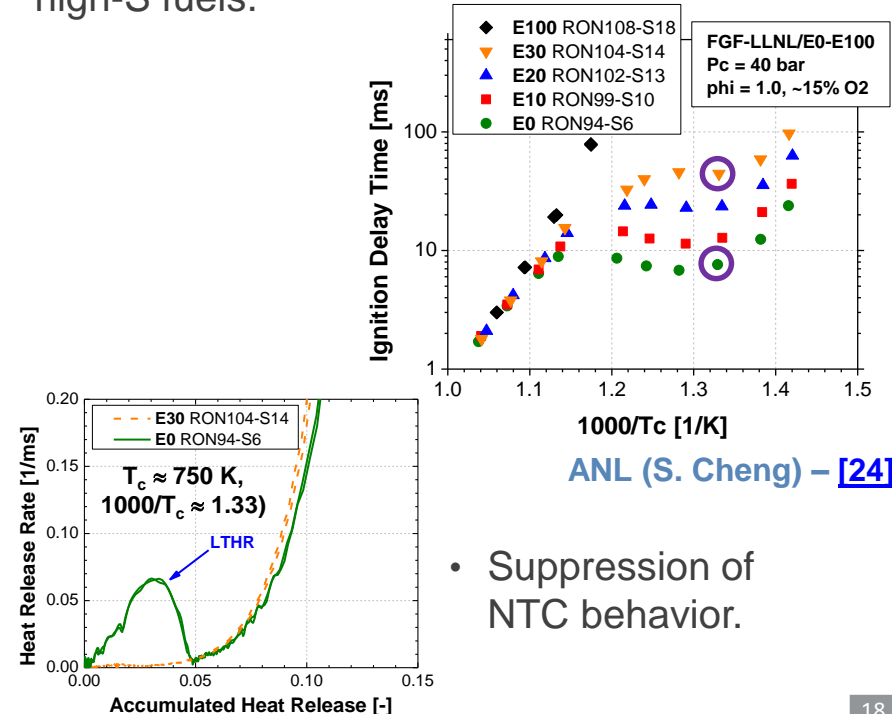


SNL (D. Vuilleumier) - [5]

# Fundamental Measurements of Fuel Autoignition



- RCM experiments at ANL show that autoignition becomes more sensitive to changes of charge temperature ( $T_c$ ) for high-S fuels.



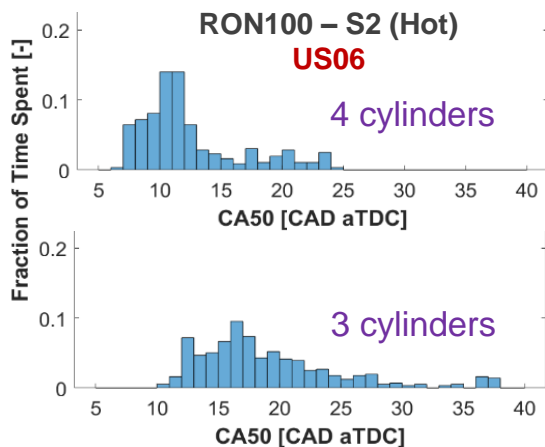
ANL (S. Cheng) – [24]

- Suppression of NTC behavior.

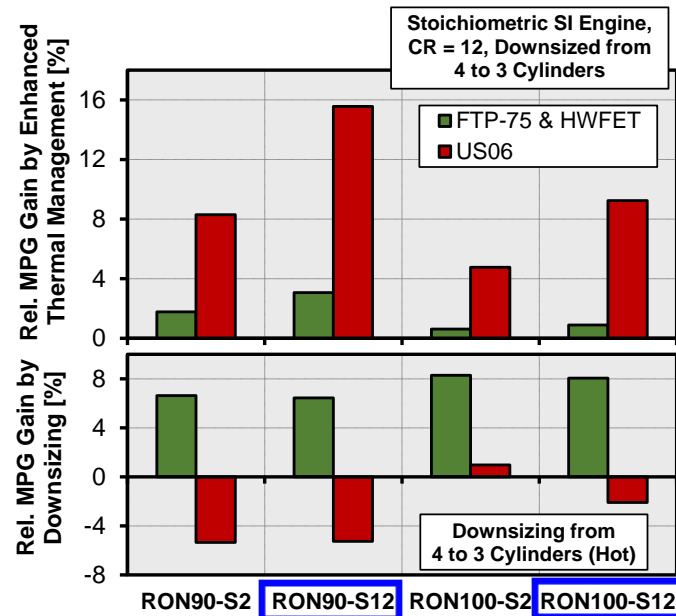
# Fuel Effects on the Benefit of Enhanced Thermal Management



- Downsizing provides FE benefits for FTP-75 & HWFET, but not for US06.
  - Higher IMEP  $\Rightarrow$  More knock limited.



- Autonomie predicts that enhanced thermal management provides most benefit for more aggressive driving (US06).

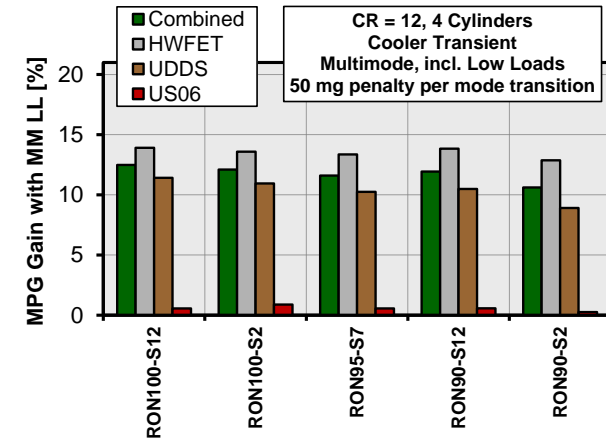
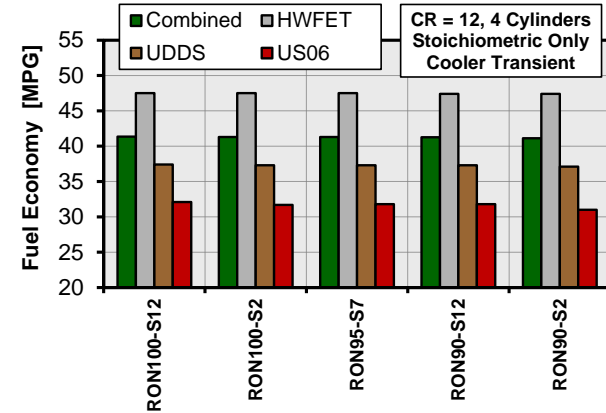
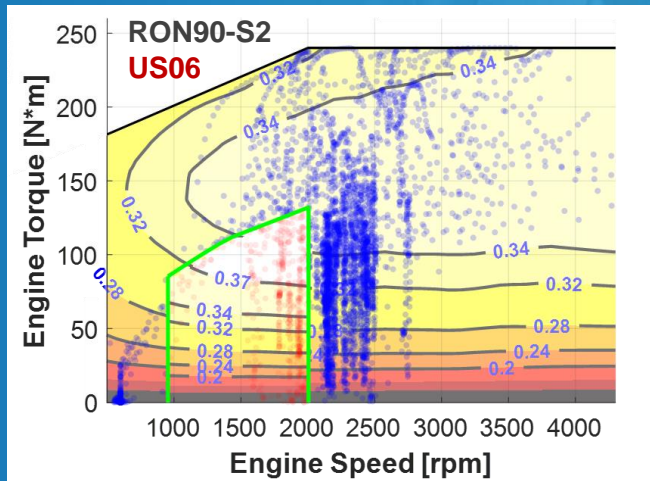


- Here, the **S=12 fuels** provide greatest benefit.

# Weak Fuel Effects for Cool Stoichiometric Operation - Benefit of Multimode Varies with Drive Cycle and Fuel Type



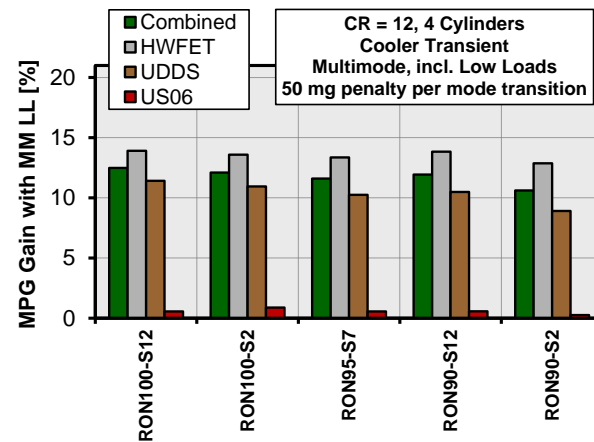
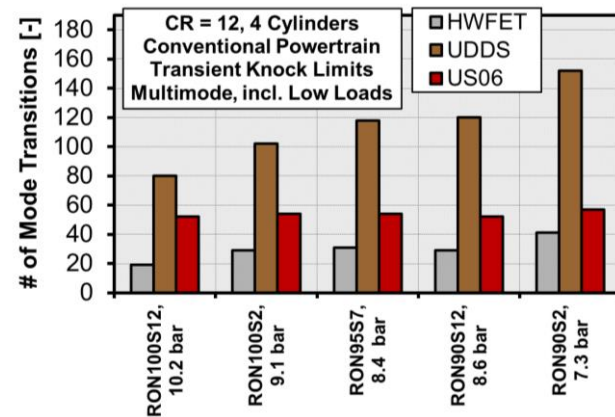
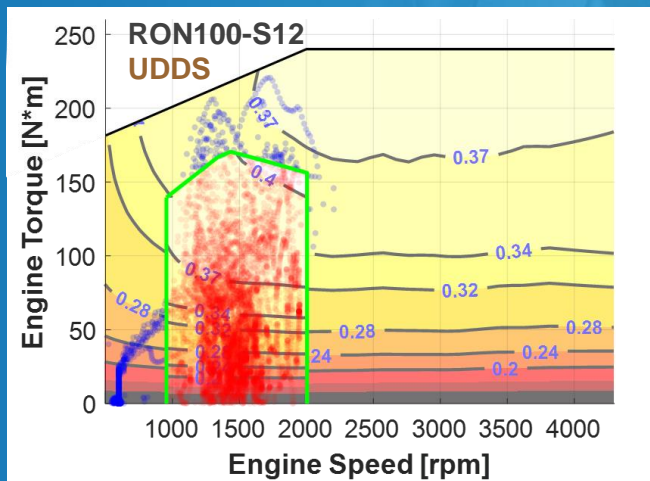
- Stoichiometric; only most aggressive US06 shows a benefit of increased RON & S.
- Boosted SI Merit Function assumes CR adjustment with fuel type, here CR = 12.
- Multimode shows essentially no benefit for US06 which uses higher engine speeds.



# Substantial Fuel-Economy Benefits from Multimode Operation for HWFET & UDDS



- Multimode operation provides 9 – 14% MPG Gains for HWFET & UDDS cycles.
- Mode switching most frequent for UDDS.
- Here, the higher SACI load limit of high-  
RON high-S fuels provides benefits.



# Summary

- Multimode engine operation can provide fuel-economy gains of more than 10% for a conventional powertrain.
- For SACI, increased RON & S enable higher loads.
  - Reduces the mode-switching frequency.
  - Octane appetite of SACI is aligned with that of Boosted SI.
- To a large degree, the Octane Index framework is applicable to LD ACI.
- Emissions regulations must be met.
- Lean operation can result in excessive formation of  $\text{NO}_x$ , HC, CO and PM.

# Future Work\*



- Assess the benefits of multimode engine operation for a hybridized powertrain.
- Determine mode-switching schemes that minimize fuel penalties.
- Determine the role of the fuels' Heat of Vaporization (HoV) on SACI & ACI.
- Assess how bioblendstocks affect HoV, especially for +30% blend levels.
- Investigate how improved mixture formation can reduce engine-out emissions for ACI.
- Assess the use of advanced lean aftertreatment and potential synergies with future fuels.

\* Any proposed future work is subject to change based on funding levels.

# Selected Multimode Publications – SNL & ANL



1. M. Sjöberg and W. Zeng, “Combined Effects of Fuel and Dilution Type on Efficiency Gains of Lean Well-Mixed DISI Engine Operation with Enhanced Ignition and Intake Heating for Enabling Mixed-Mode Combustion”, SAE Int. J. Engines 9(2):750-767, 2016, <https://doi.org/10.4271/2016-01-0689>
2. W. Zeng and M. Sjöberg, “Utilizing boost and double injections for enhanced stratified-charge direct-injection spark-ignition engine operation with gasoline and E30 fuels”, International Journal of Engine Research, Vol 18, Issue 1-2, pp. 131 – 142, 2017, <https://doi.org/10.1177/1468087416685512>
3. M. Sjöberg, X. He, “Combined effects of intake flow and spark-plug location on flame development, combustion stability and end-gas autoignition for lean spark-ignition engine operation using E30 fuel”, International Journal of Engine Research, Vol 19, Issue 1, pp. 86 – 95, 2018, <https://doi.org/10.1177/1468087417740290>
4. C.P. Ding, M. Sjöberg, D. Vuilleumier, D.L. Reuss, X. He, and B. Böhm, “Fuel-film thickness measurements using refractive index matching in a stratified-charge SI engine operated on E30 and alkylate fuels”, Exp Fluids (2018) 59: 59, <https://doi.org/10.1007/s00348-018-2512-5>
5. D. Vuilleumier, X. Huan, T. Casey and M. Sjöberg, “Uncertainty Assessment of Octane Index Framework for Stoichiometric Knock Limits of Co-Optima Gasoline Fuel Blends”, SAE International Journal of Fuels and Lubricants 11(3):247–269, 2018, <https://doi.org/10.4271/04-11-03-0014>
6. X. He, Y. Li, M. Sjöberg, D. Vuilleumier, C.P. Ding, F. Liu and X. Li, “Impact of coolant temperature on piston wall-wetting and smoke generation in a stratified-charge DISI engine operated on E30 fuel”, Proceedings of the Combustion Institute 37(4): 4955-4963, 2019, <https://doi.org/10.1016/j.proci.2018.07.073>
7. C.P. Ding, D. Vuilleumier, N. Kim, D.L. Reuss, M. Sjöberg, and B. Böhm, “Effect of engine conditions and injection timing on piston-top fuel films for stratified direct-injection spark-ignition operation using E30”, International Journal of Engine Research, Vol. 21:2, 2019, <https://doi.org/10.1177/1468087419869785>
8. Z. Hu, J. Zhang, M. Sjöberg, and W. Zeng, “The Use of Partial Fuel Stratification to Enable Stable Ultra-lean Deflagration-based SI Engine Operation with Controlled End-gas Autoignition of Gasoline and E85”, International Journal of Engine Research, 2020; 21(9):1678-1695, <https://doi.org/10.1177/1468087419889702>
9. N. Kim, D. Vuilleumier, X. He, and M. Sjöberg, “Ability of Particulate Matter Index to describe sooting tendency of various gasoline formulations in a stratified-charge spark-ignition engine”, Proceedings of The Combustion Institute 38 (2021): 5791–5799, <https://doi.org/10.1016/j.proci.2020.06.173>
10. J. Hwang, L. Weiss, I.K. Karathanassis, P. Koukouvinis, L.M. Pickett, S.A. Skeen, “Spatio-temporal identification of plume dynamics by 3D computed tomography using engine combustion network spray G injector and various fuels”, Fuel 280, 2020, <https://doi.org/10.1016/j.fuel.2020.118359>.
11. C. Xu, S. Som, M. Sjöberg, “Large Eddy Simulation of Lean Mixed-Mode Combustion Assisted By Partial Fuel Stratification in a Spark-Ignition Engine”, Journal of Energy Resources Technology 143 (2021), <https://doi.org/10.1115/1.4050588>
12. C. Tornatore and M. Sjöberg, “Optical Investigation of a Partial Fuel Stratification Strategy to Stabilize Overall Lean Operation of a DISI Engine Fueled with Gasoline and E30”, Energies, 2021; 14(2):396, <https://doi.org/10.3390/en14020396>
13. C. Xu, P. Pal, X. Ren, M. Sjöberg, N. Van Dam, Y. Wu, T. Lu, M. McNenly, S. Som, “Numerical Investigation of Fuel Property Effects on Mixed-Mode Combustion in a Spark-Ignition Engine”, Journal of Energy Resources Technology 143 (2021), <https://doi.org/10.1115/1.4048242>
14. N. Kim, D. Vuilleumier and M. Sjöberg, “Effects of Injection Timing and Duration on Fuel-Spray Collapse and Wall-Wetting in a Stratified Charge SI Engine,” SAE Technical Paper 2021-01-0544, 2021, <https://doi.org/10.4271/2021-01-0544>
15. C. Xu, M. Ameen, P. Pal, S. Som, “Direct Numerical Simulation of Partial Fuel Stratification Assisted Lean Premixed Combustion for Assessment of Hybrid G-Equation/Well-Stirred Reactor Model”, ICEF2021-67835, Proceedings of the ASME 2021 Internal Combustion Engine Division Fall Technical Conference, submitted.

# Selected Multimode Publications – ORNL, LLNL & ANL



16. T.R. Powell, J.P. Szybist, F. Dal Forno Chuahy, S.J. Curran, J. Mengwasser, A. Aradi and R. Cracknell, "Octane Index Applicability over the Pressure-Temperature Domain", *Energies* 2021, 14, 607.  
<https://doi.org/10.3390/en14030607>
17. J.P. Szybist, D.A. Splitter, "Impact of Engine Pressure-Temperature Trajectory on Autoignition for Varying Fuel Properties," *Applications in Energy and Combustion Science*, 2020, 1:100003.  
<https://doi.org/10.1016/j.jaecs.2020.100003>
18. F. Chuahy, T. Powell, S.J. Curran and J.P. Szybist, "Impact of fuel chemical function characteristics on spark assisted and kinetically controlled compression ignition performance focused on multi-mode operation," *Fuel*, 2021, 229(1), 120844. <https://doi.org/10.1016/j.fuel.2021.120844>
19. F. Chuahy, M. Moses-DeBusk, S.J. Curran, J.M. Storey and S.W. Wagnon, "The effects of distillation characteristics and aromatic content on low-load gasoline compression ignition (GCI) performance and soot emissions in a multi-cylinder engine," *Fuel*, 2021, 229(1),  
<https://doi.org/10.1016/j.fuel.2021.120893>
20. T. Powell and J.P. Szybist "Fuel Effects on Advanced Compression Ignition Load Limits," SAE Technical Paper, Fall PFL Conference 2021, Submitted.
21. S. Cheng, S.S. Goldsborough, C. Saggese, S. Wagnon and W.J. Pitz, "New Insights into Fuel Blending Effects: Intermolecular Chemical Kinetic Interactions Affecting Autoignition Times and Intermediate-Temperature Heat Release," *Combustion and Flame* (2021), Accepted.
22. H. Kwon, S. Lapointe, K. Zhang, S.W. Wagnon, W.J. Pitz, J. Zhu, C.S. McEnally, L.D. Pfefferle and Y. Xuan, "Sooting Tendencies of 20 Bio-Derived Fuels for Advanced Spark-Ignition Engines," *Fuel* 276 (2020),  
<https://doi.org/10.1016/j.fuel.2020.118059>
23. S. Lapointe, Y. Xuan, H. Kwon, R.A. Whitesides and M.J. McNenly, "A computationally-efficient method for flamelet calculations", *Combustion and Flame* 221 (2020) 94-102, <https://doi.org/10.1016/j.combustflame.2020.07.035>
24. S. Cheng, C. Saggese, D. Kang, S.S. Goldsborough, S.W. Wagnon, G. Kukkadapu, K. Zhang, M. Mehl and W.J. Pitz, "Autoignition and Preliminary Heat Release of Gasoline Surrogates and Their Blends with Ethanol at Engine-Relevant Conditions: Experiments and Comprehensive Kinetic Modeling", *Combustion and Flame* 228 (2021) 57-77,  
<https://doi.org/10.1016/j.combustflame.2021.01.033>
25. A. Shah, D. Kang, S. Goldsborough and T. Rockstroh, "Utilizing Static Autoignition Measurements to Estimate Intake Air Condition Requirements for Compression Ignition in a Multi-Mode Engine - Engine and RCM Experimental Study," SAE Technical Paper 2019-01-0957, 2019,  
<https://doi.org/10.4271/2019-01-0957>
26. D. Kang, A. Shah, T. Rockstroh and S. Goldsborough, "Utilizing Static Autoignition Measurements to Estimate Intake Air Condition Requirements for Compression Ignition in a Multi-Mode Engine - Application of Chemical Kinetic Modeling," SAE Technical Paper 2019-01-0955, 2019,  
<https://doi.org/10.4271/2019-01-0955>
27. A. Shah, S. Cheng, D.E. Longman, S.S. Goldsborough, T. Rockstroh, "An experimental study of uncertainty considerations associated with predicting auto-ignition timing using the Livengood-Wu integral method", *Fuel* 286:1, 2021, <https://doi.org/10.1016/j.fuel.2020.119025>
28. A. Shah, A. Hoth, C.P. Kolodziej, T. Rockstroh, "Gasoline fuels properties for multi-mode operation – Observations in a GDI and the CFR engine", *Fuel* 291, 2021, <https://doi.org/10.1016/j.fuel.2020.119680>